# The Advent of Generative Chemistry.

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## Abstract

Generative adversarial networks (GANs), first published in 2014, are among the most important concepts in modern artificial intelligence (AI). Bridging deep learning and game theory, GANs are used to generate or "imagine" new objects with desired properties. Since 2016, multiple GANs with reinforcement learning (RL) have been successfully applied in pharmacology for de novo molecular design. Those techniques aim at a more efficient use of the data and a better exploration of the chemical space. We review recent advances for the generation of novel molecules with desired properties with a focus on the applications of GANs, RL, and related techniques. We also discuss the current limitations and challenges in the new growing field of generative chemistry.